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## Process Modelling and Simulation of Biochar Usage in an Electric Arc Furnace as a Substitute for Fossil Coal

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#### Abstract

Increasing demands on the electric arc furnace (EAF) with regard to sustainability and energy efficiency are leading to various technological innovations. To reduce the carbon footprint of the steel production in EAFs, fossil coal can be substituted by biochar as investigated within the GreenEAF research projects. Palm kernel shells (PKS) were used for industrial long-term trials and showed no negative impact on product quality or energy consumption and are technically feasible, but led to different reaction behaviour. For further investigations on PKS usage in the EAF, the charging of biomass is implemented in a dynamic EAF process simulation model. As one of the biggest differences of PKS in comparison to fossil coal, the chemical energy of the higher volatile content is earlier available during the heat. The model considers the chemical composition of the type of coal and distinguishes between volatiles and fixed carbon. The simulation results and measurements of the averaged off-gas composition are showing the increased reaction rate of PKS. The results are obtained with the same model parameterisation as for anthracite charging. In the future, the model will be applicable to analyse various modes of operation with regard to optimised energy and resource efficiency.

#### **1. Introduction**

The modelling and simulation of the melting process in an EAF plays an important role for the optimisation of the process. Dynamic process models can contribute to a better understanding of energy and mass transfers and thus leading to an improvement of control or mode of operation of the furnace. Increased computational capacities are leading to more complex simulation models, which are considering more and more details. As a result, current process models are including enhanced simulation of the thermochemistry, slag, radiation and the melting of the scrap to investigate and improve EAF control strategies to increase the energy and resource efficiency.<sup>[1-7]</sup>

A further development approach is the reduction of the environmental impact of the EAF and therefore the reduction of CO<sub>2</sub> emissions during the melting process. With an average coal consumption of 12 kg per ton of liquid steel, approximately 43 kg of CO<sub>2</sub> are generated per ton of liquid steel.<sup>[8]</sup> The emissions from the usage of fossil carbon as charge coal and injection coal via lances are responsible for approximately 40-70 % of the entire direct CO<sub>2</sub> emissions from the EAF.<sup>[9]</sup> Characterised as CO<sub>2</sub> neutral, biomass in form of PKS has demonstrated its capability to substitute fossil carbon usage in the EAF by trial campaigns in lab scale and industrial scale. The results showed no negative impact on the production rate or the steel quality, but different reaction behaviour was observed.<sup>[10-12]</sup> Compared to fossil carbon, Yunos et al. noticed more intensive and longer lasting gas generation of PKS in laboratory tests.<sup>[13]</sup> Off-gas measurements during industrial tests have proven that the higher volatile content of the PKS leads to increased CO contents in the EAF off-gas at an earlier stage of the process.<sup>[11, 14]</sup> Hence, the EAF operation can be improved to increase the heat transfer from the CO post combustion to the scrap and thus accelerate the scrap melting. Properly implemented process models thereby enable rapid and cheap investigations of different operation and control strategies. For this reason, a dynamic EAF process simulation model has been further developed to consider different kinds of charged coal and injection coal within the simulation to enable future investigations on the EAF operation for different carbon carriers.

The applied EAF process model for this development is based on the model published by Logar et al.<sup>[15, 16]</sup> The model was re-implemented within the software MATLAB R2016a to solve the ordinary differential equations (ODEs) of the simulation model through MATLAB internal ODE solving methods and parallel computing. This ensures the required accuracy and guarantees fast simulation results.<sup>[17]</sup> Compared to other EAF process simulation models from literature, the re-implemented model is equipped with a detailed gas phase modelling, considering all relevant gas components from EAF off-gases (CO, CO<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>, H<sub>2</sub>O, CH<sub>4</sub>).<sup>[18]</sup> Consequently, the reaction behaviour and gas production through combustion of different coal types can be modelled and validated through off-gas measurements. First simulations of the re-implemented and enhanced process model verified the capability of detailed EAF off-gas simulation through dynamic process modelling.<sup>[19, 20]</sup>

This paper describes the implementation of different carbon carriers in a dynamic process simulation model, to investigate the usage of alternative carbon carriers in EAFs. Therefore, three different compositions of coal are definable. One for injection coal and two different compositions for charged coal. This allows simulations with different coal types and coal mixtures for the charged coal. The validation is performed with data from industrial scale tests with anthracite and PKS at the 140 t DC EAF of the Georgsmarienhütte GmbH (GMH), which were performed as a part of the GreenEAF2 project funded by the RFCS. The corresponding compositions of the used coal types for charged coal and lanced coal are defined in section of the modelling description of different carbon carriers.

## 2. EAF process model description

The applied EAF process model for this research uses a holistic approach, which is based on fundamental physical and thermodynamic equations. The model was developed by Logar et al. and combines all crucial processes occurring during the melting process by means of first order ODEs.<sup>[3, 15, 16]</sup> It includes main thermal, chemical and mass transfer phenomena, e.g. chemical reactions, melting rates, energy distribution and heat transfer through radiation, conduction and convection. The overall model therefore has several modules, each describing particular phenomena. An overview about the models sub-modules and interactions is given

## by **Figure 1**.

Due to the model complexity, the EAF is divided into nine different zones and phases, which are shown in **Figure 2**. Each zone is assumed homogeneous with regard to temperature and mass distribution and physical properties. The process model was tested and validated by Logar et al. with operational data and measurement from an industrial scale EAF and offers potential for further developments due to the high degree of publication. The selected approach has its advantages compared to other modelling techniques (e.g. fuzzy or neural network): deeper understanding of the process, transferability of results, extrapolation capability and less estimated parameters. This enables the model to be used for many different EAF designs.

The dynamic process model was further developed in parallel to the re-implementation. The usage of MATLAB internal numerical ODE-solver accelerates the simulation speed and leads to increased accuracy and reproducibility of the results, independent from the integration step size.<sup>[17]</sup> Further model enhancements are related to the gas phase. While the EAF model from Logar considers CO, CO<sub>2</sub>, N<sub>2</sub> and O<sub>2</sub>, the components H<sub>2</sub>, H<sub>2</sub>O and CH<sub>4</sub> were added to the gas phase and thus enabling further reaction mechanisms to take place in the gas phase. Especially equilibrium reactions like the Boudouard reaction, the heterogeneous and homogeneous water gas shift reaction are added besides post combustion reactions of CO, H<sub>2</sub> and CH<sub>4</sub>. The achieved results of the dynamic process model for the gas phase simulation have proven the capability to perform offline off-gas simulation.<sup>[18-20]</sup>

#### **3.** Modelling the usage of different carbon carriers

To ensure highest flexibility in the simulation of different carbon carrier input into the EAF, the compositions for charge coal and injection or lance coal can be defined as model parameters. Here, the chemical components C,  $O_2$ ,  $H_2$ ,  $N_2$ ,  $H_2O$  and ash are considered and are obtainable from chemical analysis of the corresponding coals. In addition, the lower heating value can be defined or is estimated from the composition for the later calculation of reaction enthalpies. A schematic overview of the composition of coals and biochar is given by

## Figure 3.

In case of injection or lance carbon, a single composition is definable. Any kind of coal or coal mixture has to be predefined directly in the model parameters. As a mass flow into the furnace, the chemical components are directly added to the corresponding differential variables of the EAF model. In detail, it is assumed that the total amount of C of the coal, also including the C, which is part of the volatile constituents, is added to the amount of C present in the EAF. This is equivalent to the variable  $x1_{d1}=\dot{m}_{Cinj}$  in Logar's description of chemical reactions.<sup>[16]</sup> The mass flow rate of the gaseous components  $O_2$ ,  $H_2$ ,  $N_2$  and  $H_2O$ , which are contained in the volatile constituents, are directly added to the gas phase.

In contrast to the injection coal, two different types of coal compositions are definable for charged coal. This enables the simulation of charging two different kinds and amounts of coal ( $m_{coal1}$  and  $m_{coal2}$ ) for each scrap basket into the EAF. The resulting composition of the coal mixture for each component i is thereby calculated by the process model itself with the total mass of coal, calculated by **Equation (1)** and **(2)**.

$$m_{\rm coal} = m_{\rm coal1} + m_{\rm coal2} \tag{1}$$

$$x_{\text{coal}_{i}} = \frac{m_{\text{coal}_{i}} x_{\text{coal}_{i}} + m_{\text{coal}_{2}} x_{\text{coal}_{2}_{i}}}{m_{\text{coal}}}$$
(2)

For the presented use case, anthracite and PKS are chosen for the two types of charged coal. Their chemical composition and the one for injection coal are given in **Table 1**. While the composition of anthracite and lance coal is taken from former mass and energy balance investigations at GMH by Kühn, the composition of PKS was analysed in laboratory.<sup>[21]</sup> The content of  $C_{fix}$  and volatile matters (VM) for anthracite and lance coal was recalculated from the data from Kühn.<sup>[21]</sup>

For the implementation into the process model, the overall mass of coal (m<sub>coal</sub>) is divided into three masses. First: the total mass of C, also including the amount of C from volatile matters; second: the mass of ash; and third: the remaining mass, consisting of N<sub>2</sub>, H<sub>2</sub>, O<sub>2</sub> and H<sub>2</sub>O. Compared to the total mass of EAF slag of several tons, the mass of ash of approximately one to two hundred kilograms of minerals is neglected within the model and only C and all volatile matters plus water are further considered. Hence, two additional differential variables are defined in the process model to represent the mass of charged coal: a mass of pure C (m<sub>coal C</sub>) and a mass of volatiles, consisting of N<sub>2</sub>, H<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>O and an appropriate amount of C (m<sub>coal\_vol</sub>), to realise an assumed direct reaction of the oxygen content with C. As a consequence, two different rates of changes for both masses are definable as the volatiles are assumed to react faster than pure C. Similar to the volatile mater of the injection coal; the gaseous components are released to the gas phase with the significant exception for O<sub>2</sub>. The O<sub>2</sub> is released as a result of the assumed reaction with C from the coal as CO. Although O<sub>2</sub> also reacts with C to  $CO_2$  and other elements, this assumption is made on the basis of the Boudouard equilibrium for typical EAF temperatures above 1000 °C. Further reactions of the released CO in the gas phase are occurring during the simulation. The two initial masses for C and volatiles are determined according to the amount and composition of charge coal through Equation (3) and (4).

$$m_{\text{coal}\_C} = m_{\text{coal}\_C} \cdot \left( x_{\text{coal}\_C} - x_{\text{coal}\_O2} \cdot \frac{2M_{\text{C}}}{M_{\text{O2}}} \right)$$
(3)

$$m_{\text{coal\_vol}} = m_{\text{coal\_N2}} \cdot \left[ x_{\text{coal\_N2}} + x_{\text{coal\_H2}} + x_{\text{coal\_H2O}} + x_{\text{coal\_O2}} \cdot \left( 1 + \frac{2M_{\text{C}}}{M_{\text{O2}}} \right) \right]$$
(4)

As the volatiles are assumed to be transferred to the gas phase, the empirical **Equation** (5) is chosen to represent the rate of change of the volatiles.

$$\dot{m}_{\text{coal\_vol}} = -kd_{\text{vol}}m_{\text{coal\_vol}}^{0.7} \left[ 1 - \left(\frac{V_{\text{sSc}}}{V_{\text{sSc}}\left(t=0\right)}\right)^2 \right]$$
(5)

Here,  $kd_{vol}$  represents the change rate coefficient. The 0.7<sup>th</sup> power for the mass of volatiles limits the change rate at the beginning of the melting process for high amounts of volatiles while the bracket term accelerates the change rate during the advance of the process. In contrast to that, the rate of change of C consists of three mass changes according to **Equation (6)**.

$$\dot{m}_{\text{coal}\_C} = -\dot{m}_{\text{coal}\_C-L} - \dot{m}_{\text{coal}\_C-CO} - \dot{m}_{\text{coal}\_C-Boudouard}$$
(6)

Here,  $\dot{m}_{coal\_C-L}$  represents the mass transfer to the mass of carbon available for decarburization and dissolving,  $\dot{m}_{coal\_C-CO}$  represents the direct combustion of C to CO and  $\dot{m}_{coal\_C-Boudouard}$  is the reaction rate of C with CO<sub>2</sub> according to the Boudouard reaction to form CO. The first mass change rate is implemented with an empirical approach, similar to Equation (5). For the oxidation of C to CO, as given in **Equation** (7), the rate of progress r is determined with the simple reaction kinetics approach through **Equation** (8).

$$C + 0.5O_2 \to CO \tag{7}$$

$$r = k [C_C]^1 [C_{02}]^{0.5}$$
(8)

Here, k describes the temperature dependent reaction rate constant and  $C_i$  a generalised concentration according to Kee et al.<sup>[22]</sup> The Boudouard reaction in **Equation (9)** is implemented through an approach for reversible equilibrium reactions as shown by **Equation (10)**.<sup>[22]</sup>

$$CO_2 + C \rightleftharpoons 2CO$$
 (9)

$$r = k_f \prod_{i=1}^{l} \left[ C_i \right]^{\nu'_i} - k_b \prod_{i=1}^{l} \left[ C_i \right]^{\nu''_i}$$
(10)

Here,  $k_f$  and  $k_b$  are the reaction rate constants of the forward and backward reaction and  $C_i$  is the concentration of the corresponding component i. The reaction rate constants are implemented temperature dependent and are calculated according to the Gibbs energy minimization.

#### 4. Results and discussion

This section illustrates the results from the simulation of the EAF melting process with different carbon carriers in comparison with measured data. The process simulation was performed completely offline with input data from trials at the 140 t DC-EAF of GMH. This includes all input materials, electrical and chemical energy input as well as the roof and wall cooling and off-gas mass flow, which are all considered in the simulation. Selected characteristics of the furnace and the steel production are given by **Table 2**. For the hot heel of the furnace, a constant mass of 60 t was assumed for all simulations. Due to the reason that this mass is not measured, this is one of the biggest sources for deviations of the simulation results from measured process data.

The scrap is charged via two scrap baskets into the furnace. The testing included reference heats with anthracite usage in contrast to pure PKS usage for the charge coal input. At this stage of the implementation of PKS, the obtained results should validate the process models capability to simulate the melting process and the gas phase behaviour for different input materials by using the same parametrization. Therefore, the continuously measured off-gas composition and the total off-gas energy output for the two trial campaigns are compared with the corresponding simulation results.

With regard to the reference process, 149 heats out of 205 heats at the EAF were simulated and evaluated within a simulation time of approximately one hour for all heats. The number of simulated heats was reduced due to long downtimes or extraordinary tap-to-tap times at the furnace for all neglected heats. By disregarding them, the averaged results for the off-gas composition are less influenced by irregular heats. The anthracite was charged with the first scrap basket with an average specific mass of 1.1 t/heat.

In case of the PKS trials, 364 heats out of 495 heats at the EAF are simulated and evaluated within approximately two and a half hours computing time for all heats. Due to the same reason described for anthracite, heats with long downtimes or very long tap-to-tap times are not considered for further evaluation. The PKS are charged with the first scrap basket into the EAF with an average specific mass of 1.4 t/heat. The higher specific amount was chosen, to achieve an absolute heating value equal to anthracite and was therefore increased.

To evaluate the time-dependent data like the off-gas composition, the measured (meas) and simulated (sim) data for PKS and anthracite (anthr) has been averaged over the complete dataset. Consequently, the unsteadiness of single heat results is smoothed and thus making the results better comparable. Furthermore, the process time was normalised by using the tap-to-tap time of each heat.

**Figure 4** shows the averaged measured and simulated off-gas mass fractions of CO. The black lines are representing the results of the reference process with anthracite usage while the grey lines are showing the results for PKS usage. The black solid line of the measured data agrees in large areas with the black dashed line of the corresponding simulation results. Compared to anthracite, the mass fraction of CO for PKS is higher while melting the first scrap basket. This is in accordance with expectations based on the higher volatile content of PKS and an assumed higher reactivity. Here, the simulation results, which are shown by the grey dashed line, are higher than the measured data, reaching almost 48 %. During the melting of the second scrap basket, the course is more congruent between the simulated and measured results for PKS and anthracite. However, the simulated CO fraction for the PKS case is below the measured data. That means, for the simulation and together with the higher CO fraction during the first scrap basket.

The averaged off-gas mass fractions of  $CO_2$  are shown in **Figure 5**, with the same colour allocation like the curves in Figure 4. The simulated and measured courses for both cases are in the same range of magnitude. At the end of the process, the difference between measured and simulated PKS results increased to a level of 5 %. A significant difference between both carbon carriers is not clearly visible.

**Figure 6** shows the averaged off-gas mass fractions of  $N_2$  with the same colour allocation like the curves before. Due to the increased release of CO for PKS during the melting of the first scrap basket, the fraction of  $N_2$  is below the anthracite results. During the melting of the second scrap basket and the refining phase, the difference between simulated and measured data reaches approximately 10 % for both carbon carrier cases. At the end of the process, lower fractions of  $N_2$  are visible for the PKS case, due to higher CO fractions. Overall, the simulated and measured data for each case are in the same range of magnitude.

The averaged off-gas mass fraction of  $H_2$  is given by **Figure 7**. Here, a different scale is chosen due to the comparatively low mass fractions of  $H_2$  occurring during the process. The differences between measured and simulated data are obvious for both cases. Nevertheless, the case with PKS usage shows higher fractions of  $H_2$  during the melting of the first scrap basket for the measured and simulation data. This is in accordance with the expectations based on higher volatile contents for PKS and is reproduced by the simulation. Even though the difference between measured and simulated data is more significant, the absolute difference is small compared to the fractions of CO, CO<sub>2</sub> and N<sub>2</sub>.

For a further comparison of anthracite and PKS usage, the specific off-gas energy output per ton of liquid steel (ISc) is shown as boxplots in **Figure 8**. For the enthalpy, often declared as sensible heat, the simulation reproduces the calculated values from the measured data for both cases. The median values of the specific energies for PKS and anthracite are in the same range of magnitude. The simulated results for both cases are leading to higher chemical energy output, due to the increased CO output as shown by Figure 4. The biggest difference between

PKS and anthracite is visible in the variance. The upper and lower quartiles are bigger for anthracite than for PKS. This is not reproduced by the simulation and it can be assumed, that this is caused by transient behaviour, e.g. carbon accumulation in the EAF as described by Kühn.<sup>[21]</sup>

Regarding the off-gas enthalpy, the mass flow and the temperature are the most important influencing factors. For a further comparison, the measured and simulated off-gas temperature for anthracite and PKS is given in **Figure 9**. Even though the heating value of PKS and anthracite has a significant difference, the influence is not clearly visible in the measured off-gas data. Here, the energy released by thermal radiation from the electric arc has a bigger impact on the energy balance of the gas phase. Concerning the simulation results, significant temperature differences to the measured off-gas temperature are obvious. However, it has to be stated that the measured off-gas temperature is a spot measurement at the elbow while the simulated off-gas temperature is a homogeneous temperature of the whole gas phase. Nevertheless, during the first melting periods of the two scrap baskets the simulated homogeneous temperature for the PKS off-gas is below the anthracite temperature. The difference in the heating value and the volatile matter influences the gas phase simulation.

The averaged results for the temperature of the liquid melt  $T_{ISc}$  are given in **Table 3**. There is a difference of 6 K between the average measured temperatures for anthracite and PKS, which is almost negligible and due to the reason, that the tapping should always be achieved with nearly the same temperature. The average simulated temperature for anthracite shows a bigger difference to the measured temperature of 37 K while the difference between measured and simulated data is 2 K for the PKS case. That means that the PKS simulation leads to lower temperatures of the liquid melt in comparison with the anthracite simulation. The lower heating value of PKS could be a simple explanation, but it has no influence during the real process as the total amount of PKS was increased compared to anthracite to achieve equal energy input. Possible errors that have to be considered are hot and cold spot measurements at the EAF that are here compared to homogeneous temperature results from the simulation. Another influencing factor is the hot heel. For the same amount of energy to heat up two different masses, the temperature difference is lower for the bigger mass. Even though the mass of the hot heel is usually in the range of 20-70 t (see Table 2), also masses of more than 100 t were observed when the refractory of the furnace is almost worn out. For the same input energy, the final temperature of the liquid melt would be lower compared to a simulation with a smaller amount of hot heel. Further investigations under consideration of detailed masses for the hot heel are therefore necessary.

Regarding the chemical composition of the liquid melt, the results showed no significant difference between PKS and anthracite, which is in accordance with former investigations and therefore not shown within this paper.<sup>[8, 10, 11]</sup>

#### **5.** Conclusion

The dynamic process simulation of the EAF with different input materials aims to prove the models capability, to predict the EAF process behaviour over a wide range of conditions. Therefore, the same parametrization setting was chosen for the simulation of PKS and anthracite. Concerning the off-gas, the simulation results demonstrated a different behaviour between the two investigated input materials. Especially the off-gas mass fraction of CO and H<sub>2</sub> increased for PKS usage during the melting of the first scrap basket, as the PKS have a higher volatile matter content and are therefore assumed to be more reactive. Consequently, an increased usage of post-combustion oxygen during the early stages of the process is thinkable for PKS usage. If technically possible, this can lead to a higher energy release and an increased melting rate.

Even though the general off-gas behaviour for both cases is reproduced by the model, differences between the simulated and measured values for each case are still indicating further necessary process model improvements. In addition, the temperature of the liquid melt demonstrated further necessity of detailed modelling of the thermochemistry and consideration of exact hot heel masses. With regard to the chemical composition and the EAF energy balance, the simulation results showed no significant discrepancy between simulation results and measurements of PKS and anthracite.

In the future, the model will be enhanced and further developed concerning the thermochemistry and steel, slag and gas phase interaction. Followed by another validation process, the dynamic process simulation model will be applicable to analyse and investigate different modes of operation and input materials to improve the energy and resource efficiency.

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Figure 1. Schematic overview of the dynamic EAF process model



Figure 2. Zones and phases of the EAF process model



Figure 3. Schematic composition of coals and biochar



Figure 4. Off-gas mass fraction of CO



Figure 5. Off-gas mass fraction of CO<sub>2</sub>



Figure 6. Off-gas mass fraction of N<sub>2</sub>



Figure 7. Off-gas mass fraction of H<sub>2</sub>



Figure 8. Measured and simulated off-gas energies for anthracite (left) and PKS (right)



Figure 9. Measured and simulated off-gas temperatures

	C <sub>total</sub> [%]	C <sub>fix</sub> [%]	VM [%]	N2 [%]	H2 [%]	O2 [%]	H2O [%]	Ash [%]	Lower heating value [MJ kg <sup>-1</sup> ]
Anthracite	81	80	9	5	3	0	6	5	33.5
PKS	53	25	64	1	6	29	8	3	19.5
Lance coal	93	83	11	0	1	0	2	4	31.8

**Table 1.** Composition of anthracite, PKS and injection coal in mass-% (an)

Table 2. Characteristic data of the 140 t DC EAF at GMH  $^{[11]}$ 

Property	Data
Tapping weight	142 t
Scrap input	150 t, 2 baskets
Hot Heel	20-70 t
Installed Power	130 MVA
Oxygen usage	38 m³/t
Natural gas usage	4 m <sup>3</sup> /t
Carbon usage	16 kg/t

**Table 3.** Temperature of the liquid melt  $T_{1Sc}$ 

	Anthracite	PKS
T <sub>lSc,meas</sub> [K]	1886	1892
$\overline{T_{ISc,sim}}$ [K]	1923	1894
s <sub>T_lSc</sub> [K]	55,8	48
$\overline{\Delta T_{lSc}}$ [K]	37	2
$\left \Delta T_{lSc}\right $ [K]	55	39